Sharp signature of DDW quantum critical point in the Hall coefficient of the cuprates

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We study the behavior of the Hall coefficient, R_H, in a system exhibiting $d_{x^2-y^2}$ density-wave (DDW) order in a regime in which the carrier concentration, x, is tuned to approach a quantum critical point at which the order is destroyed. At the mean-field level, we find that $n_{\text{Hall}} = 1/R_H$ evinces a sharp signature of the transition. There is a kink in n_{Hall} at the critical value of the carrier concentration, x_c; as the critical point is approached from the ordered side, the slope of n_{Hall} diverges. Hall transport experiments in the cuprates, at high magnetic fields sufficient to destroy superconductivity, should reveal this effect.

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There has recently been great interest in the possibility that the "pseudogap" state of the cuprates is, in fact, an ordered broken-symmetry state [1]. The interplay between this ordered state and superconductivity is conjectured to lead to the suppression and eventual demise of superconductivity at low dopings. At a critical doping, x_c, which is near – but not necessarily precisely at – optimal doping, the order associated with the pseudogap is expected to evaporate. In underdoped cuprates, the two orders are expected to coexist.

An interesting way to establish the reality of this new order, which is hypothesized to be a $d_{x^2-y^2}$ density-wave [2] (DDW), is to destroy the superconductivity in the nearby region of the phase diagram [3]. If the pseudogap is due to this order, it will survive, but if, on the other hand, the pseudogap were due to superconducting fluctuations, it would collapse. The experiments by Boebinger and his collaborators in which superconductivity is destroyed by 60 T pulsed fields are ideally suited for this purpose [4]. The effect of such magnetic fields, which are high enough to destroy superconductivity, has been shown to have little effect on DDW order [5], ensuring conditions under which DDW order can be studied in its pristine form. In particular, the transition between the DDW at lower carrier concentration to the "normal" state at higher carrier concentration can be studied at asymptotically low temperatures. An important question is whether or not this transition leaves a sharp signature in a measurable property, with emphasis on the word sharp. Boebinger and his collaborators [6] have addressed precisely this question by measuring the low-temperature Hall constant R_H or, rather, its inverse, $n_{\text{Hall}} = 1/R_H = (\sigma_{xx})^2/\sigma_{xy}$. In conventional Drude theory, it is equal to ne/B, where n is the carrier density, e is the electron charge, and B is the applied magnetic field. Preliminary measurements [6] indicate indeed a sharp signature in n_{Hall} at a carrier concentration $x_c \sim 0.15$. While these difficult and important experiments need to be firmly established, we wish to discuss this question theoretically from the DDW perspective. Thus, experimental results provide the context and the motivation for our theoretical work.

We study the Hall number, n_{Hall}, close to the quantum phase transition at zero temperature. The theoretical framework is an effective Hartree-Fock Hamiltonian that captures the broken symmetry of the DDW order. The contribution of nodal quasiparticles, arising from this Hamiltonian, to electrical and thermal transport was previously studied, and it was shown how they can be used to detect DDW order [7]. However, near the quantum critical point at $x = x_c$, where DDW order disappears, the DDW gap is small, and it is not sufficient to focus solely on the nodal quasiparticles; quasiparticles far from the nodes are equally important. In this paper, we report the results of a calculation which takes into account all of the relevant parts of the Fermi surface. We consider the Hall coefficient in linear response theory, using the Kubo formulae. We find that the Kubo formulae lead to the same results as the Boltzmann equation in the weak scattering limit, unlike in the case of nodal quasiparticles, where the Boltzmann equation cannot be naively used. Consistent with the Hartree-Fock effective Hamiltonian, we assume a mean-field dependence of the magnitude of the zero-temperature DDW gap, $\Delta(x)$, on $x_c - x$, $\Delta(x) = \Delta_0(x_c - x)^{1/2}$, for $x < x_c$; here on, we will drop the argument of $\Delta(x)$, if there is no danger of confusion. We find a kink in n_{Hall} against x. As $x \to x_c^-$, the slope of $n_{\text{Hall}}(x)$ diverges; for $x \to x_c^+$, the slope remains finite. As we discuss below, the change in the slope is due to the contribution of the "hot spots", where the Fermi surface crosses the reduced Brillouin zone (or magnetic zone) boundary [8].

It is clear that fluctuation effects can not be neglected at the quantum critical point as $x \to x_c$. On dimensional grounds, however, there is some reason for believing that the quantum critical region is very narrow and is of order $(\Delta_0/E_F)^2$, where E_F is the Fermi energy. It would indeed be very difficult to explore the critical region, as it would require preparing samples with an extraordinary degree of control of doping. Thus, the choice of the mean-field critical exponent is eminently reasonable. As an *ad hoc* procedure, we have also discussed other

possible dependences of Δ on $x_c - x$, only because such choices have appeared in the literature [9]. We want to warn the reader, however, that these choices are merely empirical and no theoretical justifications can be offered. The actual theoretical problem of incorporating fluctuations at the quantum critical point is more complex, which is squarely beyond the scope of the present paper; we further remark on this issue later.

First, we use the Kubo formula to derive the conductivity and Hall conductivity of a system of electrons with DDW order, assuming that the only source of scattering is impurities. 'Residual' interactions which remain after the development of DDW order are neglected. We begin with the mean field Hamiltonian for the DDW state:

$$H = \sum_{\mathbf{k},\alpha}[(\epsilon_{\mathbf{k}} - \mu)\,c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} + i\Delta_{\mathbf{k}}c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k+Q}\alpha} + \text{h. c.}] \quad (1)$$

where $c_{\mathbf{k}}$ is the annihilation operator for an electron of spin α in the z-direction and momentum $\mathbf{k}$. The single particle spectrum on the square lattice with nearest-neighbor hopping t and next-neighbor hopping t' is $\epsilon_{\mathbf{k}} = 4t'\cos k_x \cos k_y - 2t(\cos k_x + \cos k_y)$. $\Delta_{\mathbf{k}} = \Delta(\cos k_x - \cos k_y)$ is the d- wave order parameter of DDW state and the vector $\mathbf{Q} = (\pi, \pi)$. We have set the lattice spacing to be unity. We can express the Hamiltonian in terms of a 2-component quasiparticle operator: $\Psi_{\mathbf{k},\alpha}^\dagger = (c_{\mathbf{k}\alpha}^\dagger, -ic_{\mathbf{k+Q}\alpha}^\dagger)$, and then diagonalize this simple 2×2 Hamiltonian, to get

$$H = \sum_{\mathbf{k},\alpha} \chi_{\mathbf{k},\alpha}^\dagger \begin{pmatrix} [E_+(\mathbf{k}) - \mu] & 0 \\ 0 & [E_-(\mathbf{k}) - \mu] \end{pmatrix} \chi_{\mathbf{k},\alpha}, \quad (2)$$

where $E_\pm(\mathbf{k}) = \epsilon_{2\mathbf{k}} \pm \sqrt{\epsilon_{1\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$; here, $\epsilon_{1\mathbf{k}} = -2t(\cos k_x + \cos k_y)$, $\epsilon_{2\mathbf{k}} = 4t'\cos k_x \cos k_y$. The two-component quasiparticle operator $\chi_{\mathbf{k}\alpha}$ is a unitarily related to $\Psi_{\mathbf{k}\alpha}$, and the sum is over the reduced Brilloun zone (RBZ).

Since the field χ is the superposition of two charge $-e$ fields, it, too, is a charge $-e$ field. Hence, the electrical current operators are given by

$$j_{x,y} = e \sum_{\mathbf{k},\alpha} \chi_{\mathbf{k}\alpha}^\dagger \begin{pmatrix} \frac{\partial E_+(k)}{\partial k_{x,y}} & 0 \\ 0 & \frac{\partial E_-(k)}{\partial k_{x,y}} \end{pmatrix} \chi_{\mathbf{k}\alpha} \quad (3)$$

In the Kubo approach, conductivities are obtained by applying weak electrical and magnetic fields to the system: $\mathbf{E} = E_0\hat{x}\cos(\omega t)$, $\mathbf{B} = q\hat{z}A_0\sin(qy)$. At the linear response level, the conductivity is given by:

$$\sigma_{xx} = \frac{1}{\omega}\text{Im}\Pi_2(i\omega_n \to \omega + i\delta, \mathbf{q} = 0, T) \quad (4)$$

where $\Pi_2(i\omega_n, \mathbf{q}, T) = \int_0^\beta d\tau e^{i\omega_n\tau} < T_\tau j_x(\mathbf{q}, \tau)j_x(\mathbf{q}, \tau) >$ is the Fourier transform of the imaginary time-ordered current-current correlation function, and ω_n is the Matsubara frequency (β is the inverse temperature). The Hall conductivity is given by [10]:

$$\sigma_{xy}(\omega, T) = \lim_{q \to 0} \frac{B}{\omega q} \text{Re}\Pi_3(i\omega_n \to \omega + i\delta, q\hat{y}, T), \quad (5)$$

where

$$\Pi_3(i\omega_n, \mathbf{q}, T) = $$
$$\int_0^\beta d\tau d\tau' e^{i\omega_n\tau} < T_\tau j_y(\mathbf{q}, \tau)j_x(0, 0)j_y(-\mathbf{q}, \tau') > \quad (6)$$

In the limit of large scattering time, τ_s, we make the usual approximations [11], and taking $q \to 0$, $\omega \to 0$ limits, we get

$$\sigma_{xy} = e^3 B \tau_s^2 \int \frac{d^2k}{(2\pi)^2}\Big[\frac{\partial E_+(k)}{\partial k_x}\frac{\partial E_+(k)}{\partial k_y}\frac{\partial^2 E_+(k)}{\partial k_x \partial k_y} - $$
$$\Big(\frac{\partial E_+(k)}{\partial k_x}\Big)^2\frac{\partial^2 E_+(k)}{\partial k_y^2}\Big]\delta(E_+(k) - \mu) + (E_+ \to E_-), \quad (7)$$

and

$$\sigma_{xx} = e^2\tau_s \int \frac{d^2k}{(2\pi)^2}\Big(\frac{\partial E_+(k)}{\partial k_x}\Big)^2\delta(E_+(k) - \mu)$$
$$+ (E_+ \to E_-) \quad (8)$$

These are precisely the same formulae that are obtained from the Boltzmann equation [12].

With formulae (7) and (8) in hand, we can proceed to calculate the Hall coefficient. Above the critical hole concentration ($x_c \sim 0.2$), there is no DDW order, and n_{Hall} is obtained from the same formulae, but with the quasiparticle dispersions $E_\pm(\mathbf{k})$ replaced by the tight-binding electron band structure $\epsilon_{\mathbf{k}}$. In this case, the sign of the Hall number is determined by the curvature of the tight binding electron Fermi surface. If the Fermi surface is closed around the center of the first Brillouin zone (the Γ-point), the Hall effect will be electron-like, and n_{Hall} will be negative. On the other hand, if the Fermi surface closes around the corners of the zone (the M-points), n_{Hall} is positive, and the response is hole-like. Band structure calculations [13], corroborated by a wide spectrum of phenomenology, indicate that the latter scenario occurs in the cuprates. This is a constraining factor in our choice of parmeters.

Insofar as the behavior close to the critical point is concerned, the variation of μ is clearly smoother than the variation of Δ, and we can treat μ as constant, thereby neglecting the smooth variation of the Hall coefficient which is generated by the variation of μ with x. The results shown below correspond to $t = 0.3$ eV, $t'/t = 0.3$, $\mu = -t$, and $x_c = 0.2$. The precise value of x_c is unimportant in our calculation. Its value is non-universal and could vary between materials. For example, it is about 0.15 in Ref. [6], while it is about 0.2 in Ref. [9]. Because we hold μ constant around x_c, we will obtain a Hall coefficient, which is also a constant for $x > x_c$. Later, we will comment on the correction to this assumption. The order parameter, Δ, is assumed to scale with a mean field

exponent near the critical point: $\Delta(x) = \Delta_0(x_c - x)^{1/2}$. For a representative value, we have chosen $\Delta_0 = 0.03$ eV. We wish to emphasize that the results of our calculation are robust with respect to the choice of parameters, as long as the considerations pertaining to the hot spots described below hold. We have explicitly tested this by choosing a wide range of parameters.

Let us now analyze equations (7) and (8) close to the critical point. The formulae involve integrals over the Fermi surface of first and second derivatives of the quasiparticle dispersion. Let us first consider a typical derivative, such as $\frac{\partial E_{+\mathbf{k}}}{\partial \mathbf{k}_x}$, which appears in the integrand on the ordered side of x_c, for small values of $|x - x_c|$.

$$\frac{\partial E_{+\mathbf{k}}}{\partial \mathbf{k}_x} = -4t' \sin k_x \cos k_y -$$

$$\sin k_x \frac{\frac{\Delta^2}{4}(\cos k_x - \cos k_y) + 4t^2(\cos k_x + \cos k_y)}{[4t^2(\cos k_x + \cos k_y)^2 + \frac{\Delta^2}{4}(\cos k_x - \cos k_y)^2]^{\frac{1}{2}}} \quad (9)$$

For small values of $|x - x_c|$ on the ordered side, Δ is negligible over most of the region of integration. However, this is not true at those points on the Fermi surface where $t(\cos k_x + \cos k_y)$ is even smaller than Δ; at these points, Δ is important. This will be the case at the points where the Fermi surface crosses the RBZ boundary – the "hot spots" [8] – and finite regions $|\cos k_x + \cos k_y|/|\cos k_x - \cos k_y| < \Delta/4t$ about them. These regions of integration will give rise to a slope discontinuity in n_{Hall}.

To illustrate this, we consider the quantity (9) along the boundary of the RBZ:

$$\frac{\partial E_{+\mathbf{k}}}{\partial \mathbf{k}_x} = -4t' \sin k_x \cos k_y - \frac{\Delta}{2} \sin k_x \quad (10)$$

On the other hand, in the disordered phase for $x > x_c$, Δ is identically zero, so $\frac{\partial E_{+\mathbf{k}}}{\partial \mathbf{k}_x}$ takes the following value along the boundary of the reduced Brillouin zone:

$$\frac{\partial E_{+\mathbf{k}}}{\partial \mathbf{k}_x} = -4t' \sin k_x \cos k_y - 2t \sin k_x \quad (11)$$

Thus, in the $\Delta \to 0$ limit, this quantity has a discontinuity of order t at the RBZ edges.

Consider, now, $\frac{dn_{\mathrm{Hall}}}{d\Delta}$ for $\Delta \to 0$: $\frac{dn_{\mathrm{Hall}}}{d\Delta} = \frac{2\sigma_{xx}}{\sigma_{xy}}\frac{d\sigma_{xx}}{d\Delta} - \frac{\sigma_{xx}^2}{\sigma_{xy}^2}\frac{d\sigma_{xy}}{d\Delta}$. We would like this quantity to zeroeth order in Δ. Thus, we can take $\Delta = 0$ in the factors $\frac{2\sigma_{xx}}{\sigma_{xy}}$ and $\frac{\sigma_{xx}^2}{\sigma_{xy}^2}$. Inside the derivatives, we only need to keep the linear in Δ terms in σ_{xx} and σ_{xy}. Hence, the computation reduces to understanding the leading Δ dependence of σ_{xx} and σ_{xy}. Consider the integral of Eq. 7; the integral of Eq. 8 is similar. We can calculate (7) for Δ small as the $\Delta = 0$ value plus a correction term coming from the integral over the region around the hot spot. From (10) and (11), we see that the integrand – which is a product of three such derivatives – is finite in the $\Delta = 0$ limit. Hence, the

leading Δ dependence comes simply from the size of the integration region, $|\cos k_x + \cos k_y|/|\cos k_x - \cos k_y| < \Delta/4t$, which is $\sim t\Delta$.

Thus, we find that the leading Δ dependence as $x \to x_c^-$ is linear. As $\Delta \to 0$, this term vanishes, so the Hall constant is continuous. However, its derivative with respect to x will not vanish as $x \to x_c$. The slope of n_{Hall} (normalized to its value at x_c) will actually diverge for $x \to x_c^-$. In Fig. 1, we have plotted the calculated values of n_{Hall} with x close to x_c on either sides, with the mean-field dependence of $\Delta(x)$. As we see, the extra contribution resulting from non-zero Δ is negative.
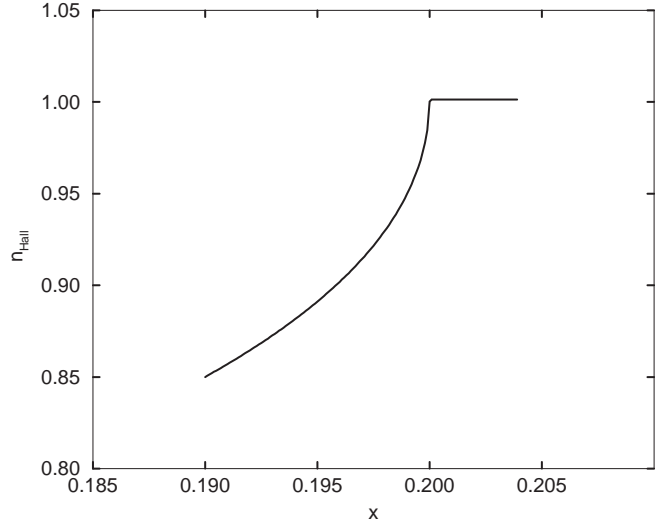

FIG. 1. The Hall number calculated as a function of doping x. Note that $\frac{dn_{\mathrm{Hall}}}{dx} \sim (x_c - x)^{-1/2}$, at the quantum critical point as $x \to x_c^-$. n_{Hall} was normalized to its value at x_c.

The effect is further illuminated by considering the evolution of the Fermi surface itself. As the system crosses from the disordered side of the transition to the DDW side, the Fermi surface becomes disconnected precisely at the hot spots. In the extreme case, $t' = \mu = 0$, where the tight-binding Fermi surface *is* the RBZ boundary, this occurs everywhere on the Fermi surface. The Fermi surface is reduced to the four nodal Fermi points even for infinitesimal Δ (it is disconnected everywhere). However, for any finite μ, t', the disconnection takes place only at the eight crossing points, the hot spots. The typical DDW band structure is shown in Fig. 2.

The nature of the discontinuity in the slope of h_{Hall} depends on the critical behavior of the DDW single-particle gap. One may wonder, what would happen if the gap behaved more generally with a critical exponent β' given by

$$\Delta(x) = \Delta_0(x_c - x)^{\beta'}? \quad (12)$$

Superficially, the slope will vary as $|x - x_c|^{\beta'-1}$ as the transition is approached from the ordered side, if we plug
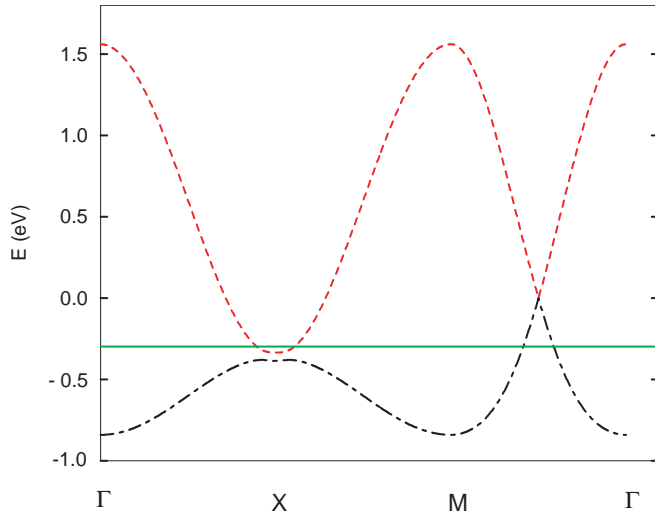
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FIG. 2. The DDW bandstructure plotted along special directions of the Brill ouin zone of the square lattice; the point group symmetry is $4mm$. The parmeters a re described in the text. The upper band is the dashed curve and the lower band is the dashed-dotted curve; the chemical potential is noted by a solid line. Note that the chemical potential lies in the upper band at the X point.

this $\Delta(x)$ in our equations. If $\beta' < 1$, as is the case in mean-field theory ($\beta' = 1/2$), then the slope will diverge as the transition is approached from the ordered side. If $\beta' = 1$, as Loram *et al.* suggests [9], then there is a finite slope discontinuity. If $\beta' > 1$, then the slope is continuous at the transition and non-analyticity only shows up in higher derivatives of n_{Hall} with respect to x. It is inconsistent, however, to use a non-mean field exponent in the context of the Hartree-Fock Hamiltonian, as the exponent $\beta' \neq 1/2$ must arise from fluctuations at the quantum critical point for which we can no longer meaningfully use the Hartree-Fock Hamiltonian, or its quasiparticle excitations. As remarked earlier, the critical region is expected to be narrow and not of relevance, given the precision of present experiments.

To go consistently beyond mean-field theory, we must not only take the correct value of β – which may be the 3D Ising exponent since the DDW order parameter breaks a Z_2 symmetry – but also consider the scattering of quasiparticles by critical fluctuations.

Although our calculation was performed for DDW order, superficially, identical behavior would be obtained in the case of any order parameter at $\mathbf{Q} = (\pi, \pi)$: there would be linear in Δ contributions originating at the hot spots. The important task in this case is to phenomenologically motivate such a order parameter transition. We find no compelling evidence for the existence of other order parameters, such as a commensurate spin-density wave, or a triplet d-density wave setting in at $x = x_c$. Hypothetical order parameters at other wavevectors could

have some signature, but it might not be linear in Δ, so these order parameters may require smaller values of β' in order to manifest themselves as kinks in n_{Hall} or else they may only show up in higher derivatives of n_{Hall}. So, it is crucial to precisely determine the experimental nature of the signature at x_c in n_{Hall}.

In a real experiment, the Hall coefficient will be measured at a finite temperature. Its value will depend on the order of the limits $\Delta \to 0$, $T \to 0$. As long as $\Delta > T$, the result of the previous section will be observed. However, if it is possible to approach very close to x_c, so that $\Delta < T$, then Δ is replaced by Δ^2/T. If $\beta' = 1/2$, a slope discontinuity remains. For $\beta' > 1/2$, the transition is rounded. To summarize, an experiment at low non-zero temperature will observe a rounding of the transition within a very small window $x_c - x < T^{1/\beta'}$.

In our calculation, we have ignored the variation of μ with x. If we allow μ to vary with x in the manner dictated by the single-particle spectrum, then the result of Fig. 1 is superposed on a large but finite sloping background. In this case, n_{Hall} will not be a constant for $x > x_c$. However, there are some indications that the chemical potential varies more slowly in the underdoped regime than one might expect [14]. At any rate, this background is non-universal and determined by separate physics from that which governs the critical properties. It is really a separate issue, and we do not attempt to model it here.

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